

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, methyl ester  
145348-22-7 | DTXSID60162991

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.87e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.18e-01

Confidence level: 3.10e-01

Nearest Neighbors from the Training Set

Image not found

2,5-Dichlorodiphenyl ether

Measured: 2.78e-06

Predicted: 9.53e-04

Image not found

Kinoprene

Measured: 1.50e-08

Predicted: 1.35e-05

Image not found

Cymiazole

Measured: 1.25e-06

Predicted: 9.28e-06

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Acenaphthene

Measured: 5.17e-04

Predicted: 1.84e-03